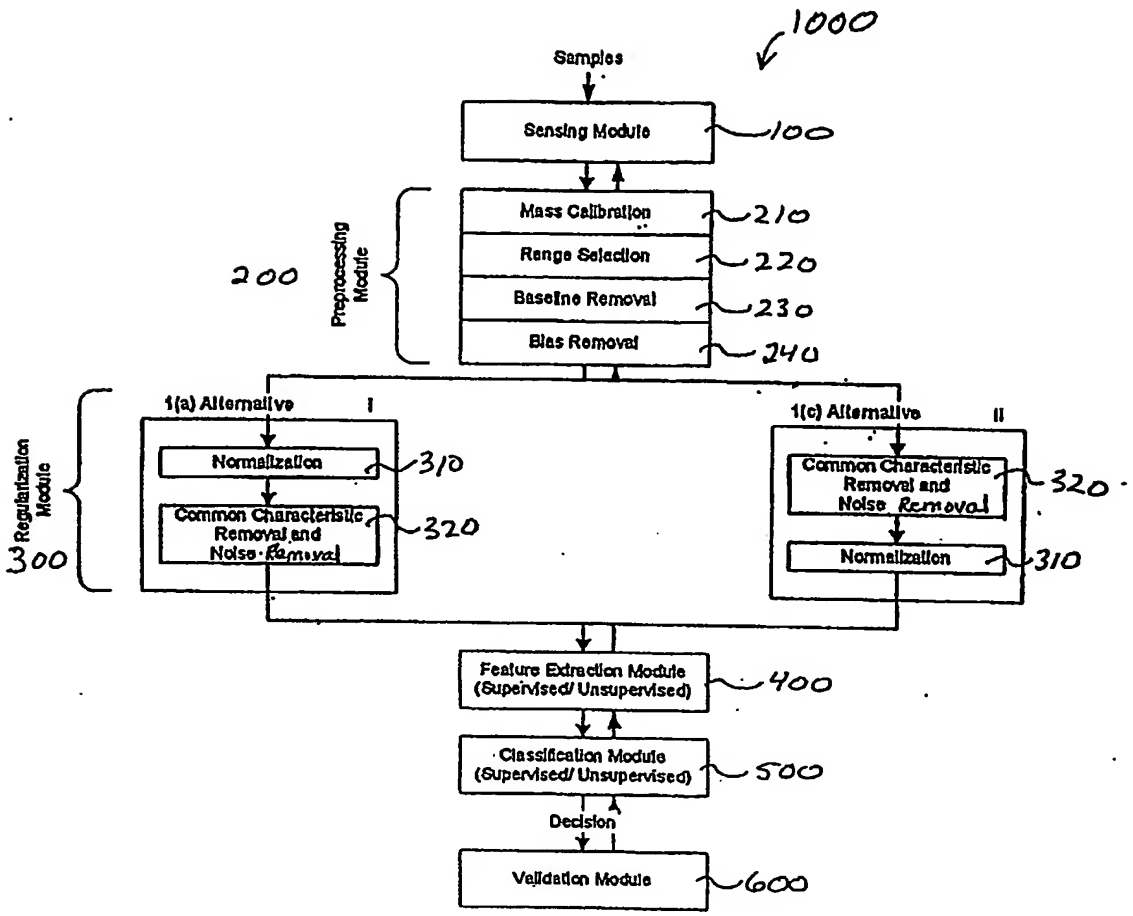

1000
Samples
Sensing Module
100
Mass Calibration
210
Range Selection
220
Baseline Removal
230
Bias Removal
240
200
Preprocessing Module
1(a) Alternative I
Normalization
310
Common Characteristic Removal and Noise Removal
320
1(c) Alternative II
Common Characteristic Removal and Noise Removal
320
Normalization
310
Regularization Module
300
Feature Extraction Module (Supervised/ Unsupervised)
400
Classification Module (Supervised/ Unsupervised)
500
Decision
Validation Module
600

FIG. 1

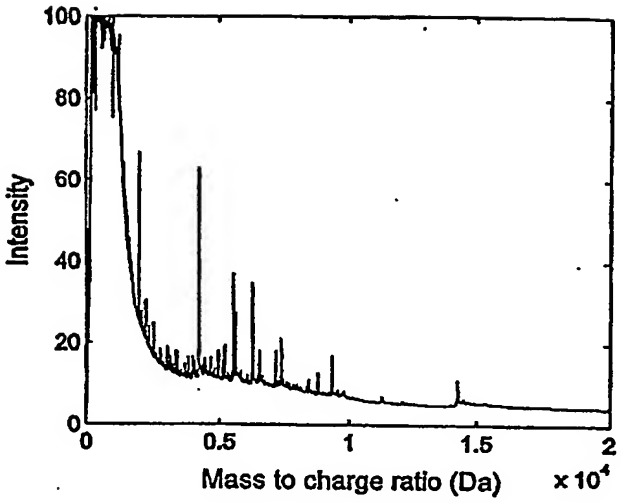

100
80
60
40
20
0
Intensity
0
0.5
1
1.5
2
Mass to charge ratio (Da)
x 10^4

FIG. 2

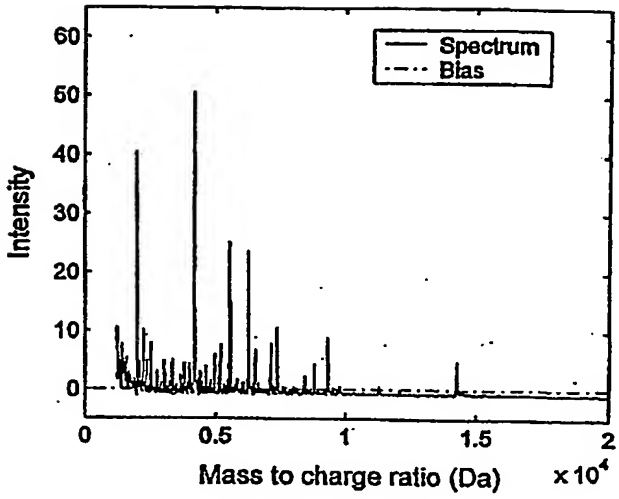
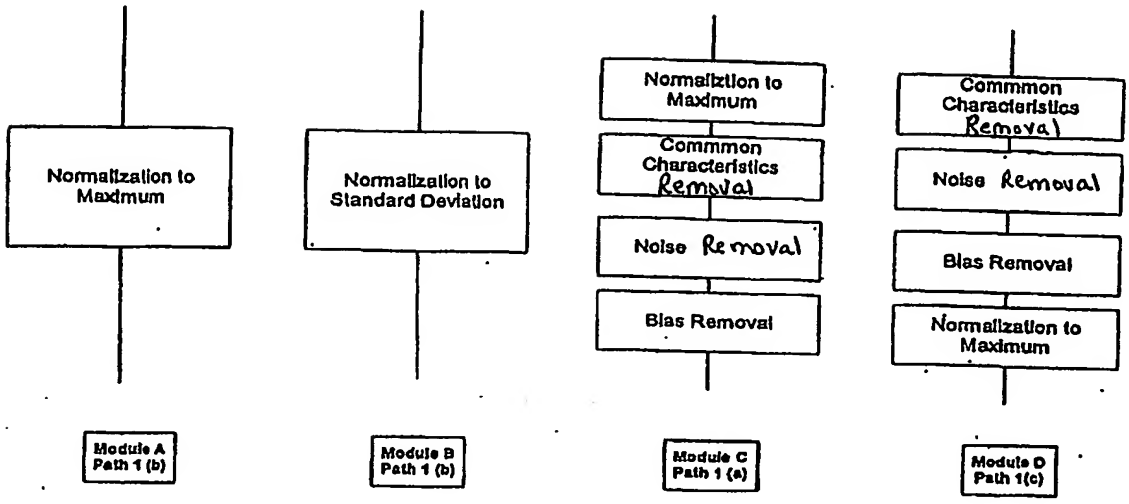

Spectrum
Bias
Intensity
60
50
40
30
20
10
0
0
0.5
1
1.5
2
Mass to charge ratio (Da)
x 10^4

FIG. 3


Normalization to Maximum
Module A Path 1 (b)
Normalization to Standard Deviation
Module B Path 1 (b)
Normalization to Maximum
Commmon Characteristics Removal
Noise Removal
Bias Removal
Module C Path 1 (a)
Commmon Characteristics Removal
Noise Removal
Bias Removal
Normalization to Maximum
Module D Path 1(c)

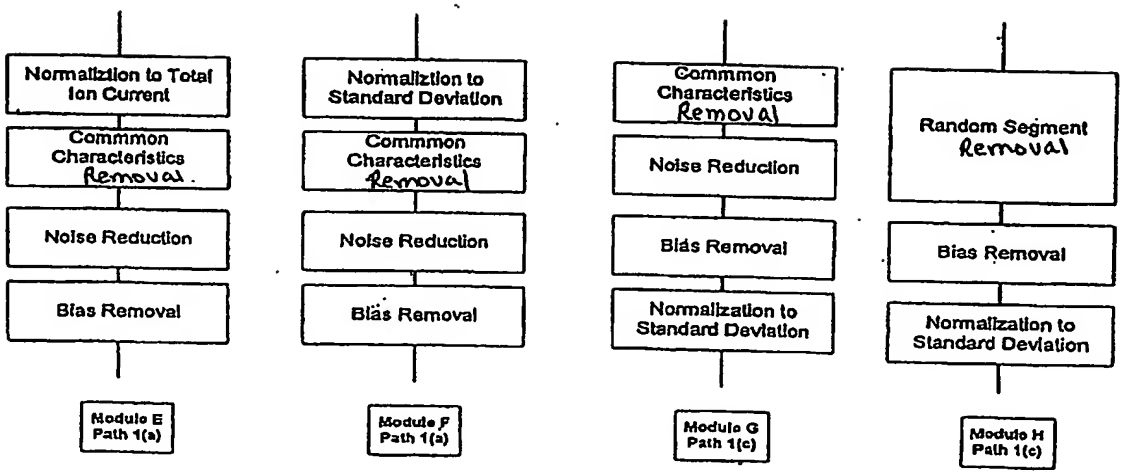

Normalization to Total Ion Current
Commmon Characteristics Removal
Noise Reduction
Bias Removal
Module E Path 1(a)
Normalization to Standard Deviation
Commmon Characteristics Removal
Noise Reduction
Bias Removal
Module F Path 1(a)
Commmon Characteristics Removal
Noise Reduction
Bias Removal
Normalization to Standard Deviation
Module G Path 1(c)
Random Segment Removal
Bias Removal
Normalization to Standard Deviation
Module H Path 1(c)

FIG. 4

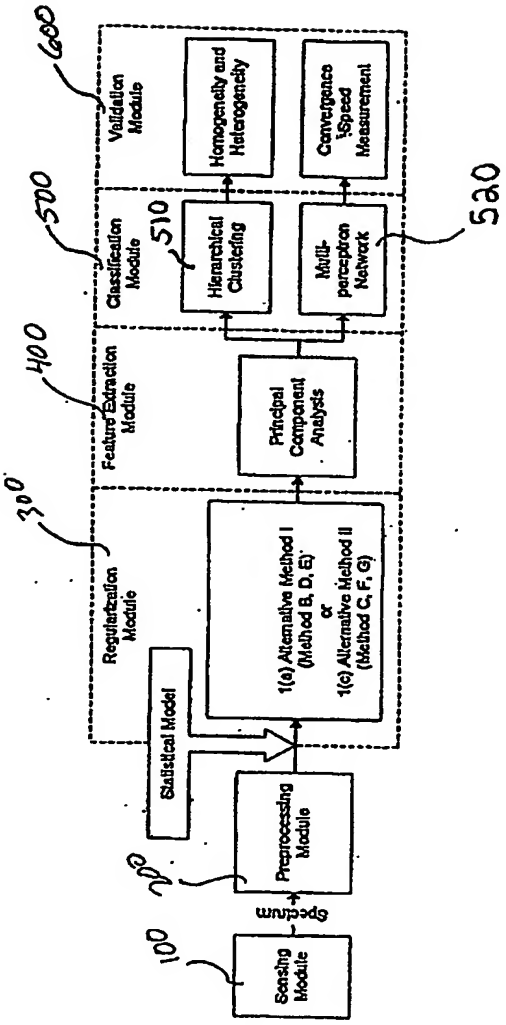

600
Validation Module
Homogeneity and Heterogeneity
Convergence Speed Measurement
500
Classification Module
510
Hierarchical Clustering
Multi-perceptron Network
520
400
Feature Extraction Module
Principal Component Analysis
300
Regularization Module
1(a) Alternative Method I (Method B, D, E) or 1(c) Alternative Method II (Method C, F, G)
Statistical Model
200
Preprocessing Module
Spectrum
100
Sensing Module

FIG. 5

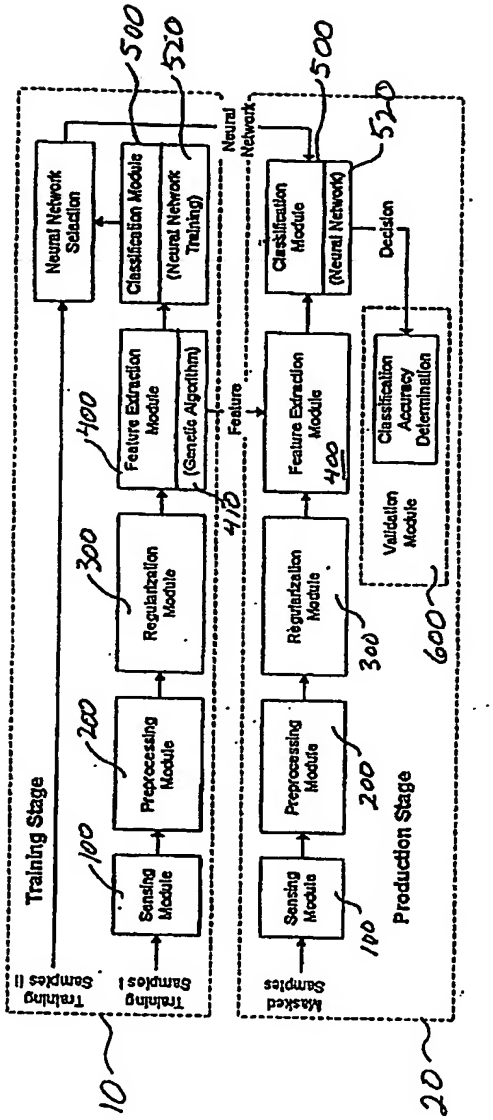

Training Stage
Training Samples I
Training Samples II
Sensing Module
Preprocessing Module
Regularization Module
Feature Extraction Module
(Genetic Algorithm)
Neural Network Selection
Classification Module
(Neural Network Training)
Feature
Neural Network
Masked Samples
Production Stage
Sensing Module
Preprocessing Module
Regularization Module
Feature Extraction Module
Classification Module
(Neural Network)
Decision
Validation Module
Classification Accuracy Determination
10
20
100
200
300
400
418
500
520
600

FIG. 6

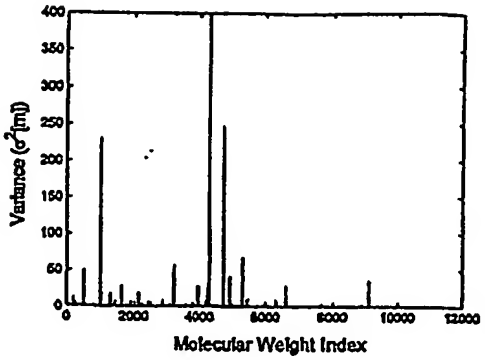



FIG. 7a

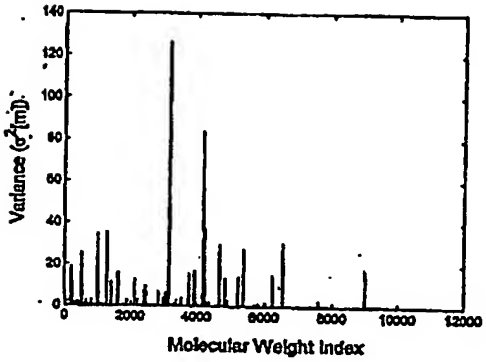



FIG. 7b

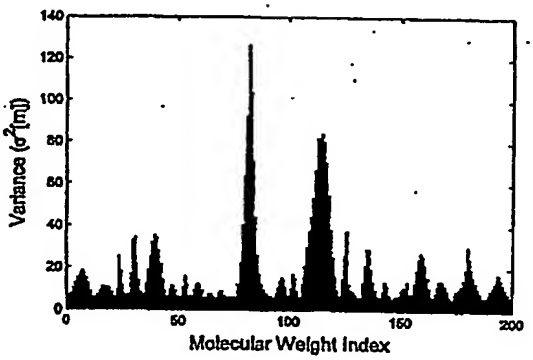



FIG. 7c

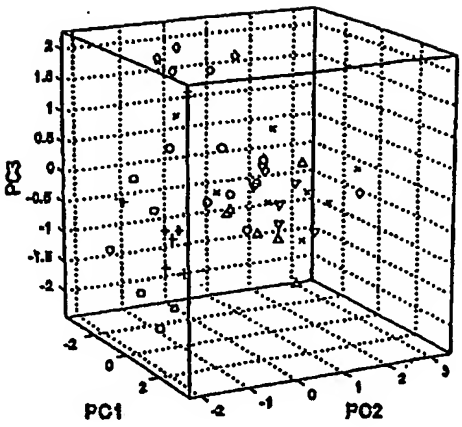



FIG. 8a

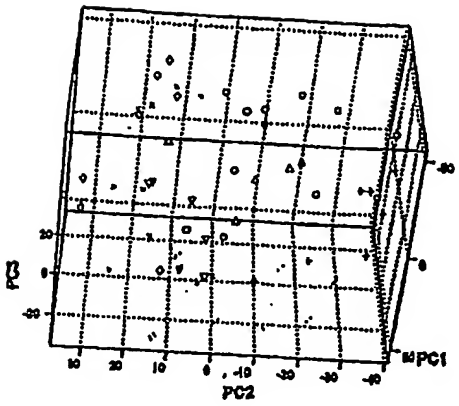



FIG. 8b

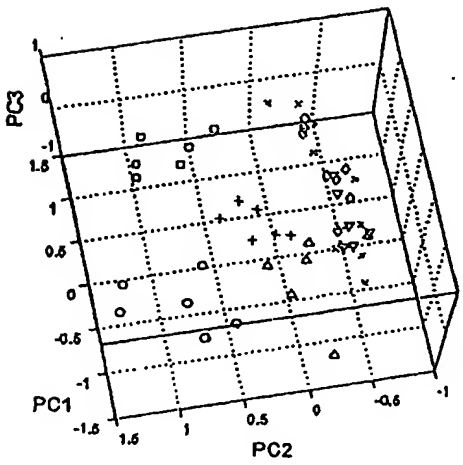



FIG. 8c

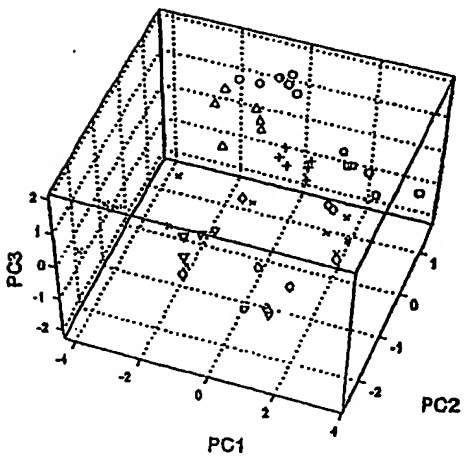



FIG. 8d

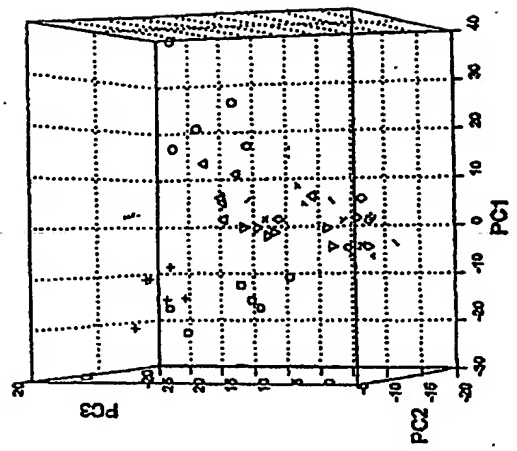



FIG. 8f

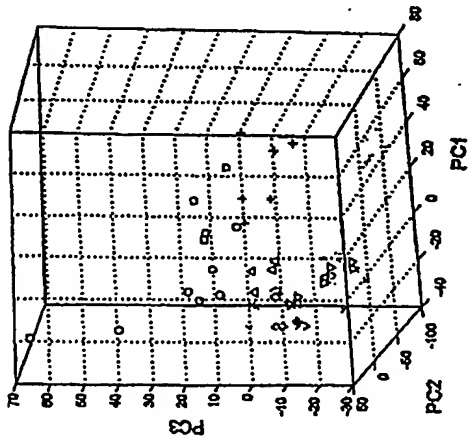



FIG. 8e

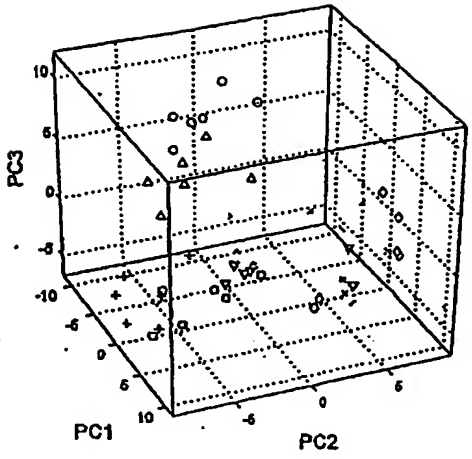



FIG. 8g

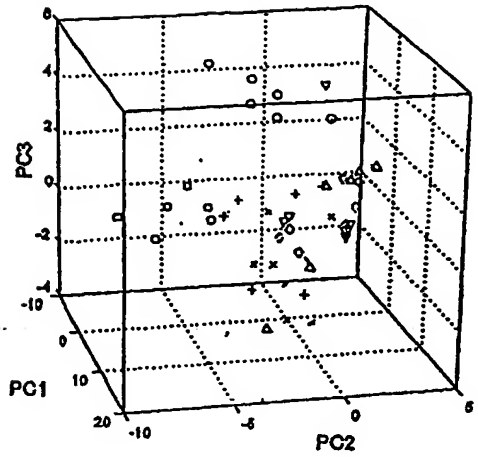



FIG. 8h

× Animal 1 (Group 1)
◇ Animal 2 (Group 1)
+ Animal 3 (Group 2)
□ Animal 4 (Group 2)
△ Animal 5 (Group 3)
▽ Animal 6 (Group 3)
○ Animal 7 (Group 4)

FIG. 8i

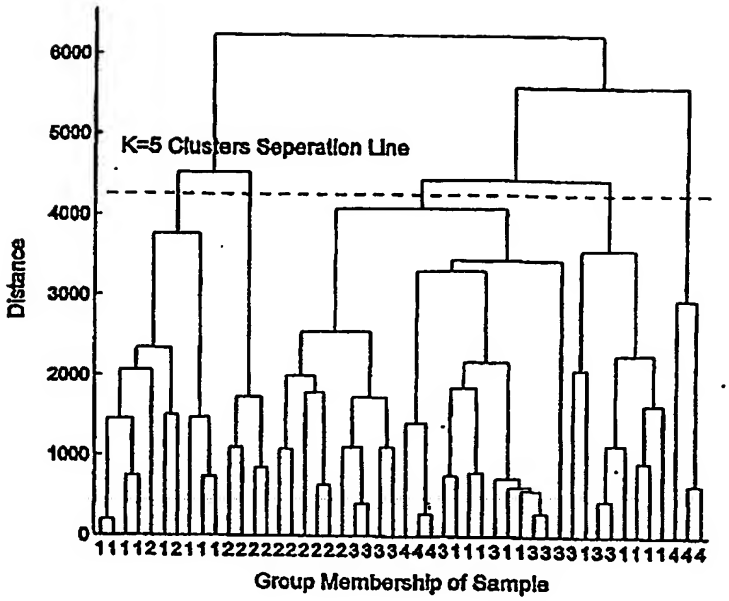

K=5 Clusters Seperation Line
Distance
6000
5000
4000
3000
2000
1000
0
11112121112222222222333344431113113333133111144 4
Group Membership of Sample

FIG. 9a

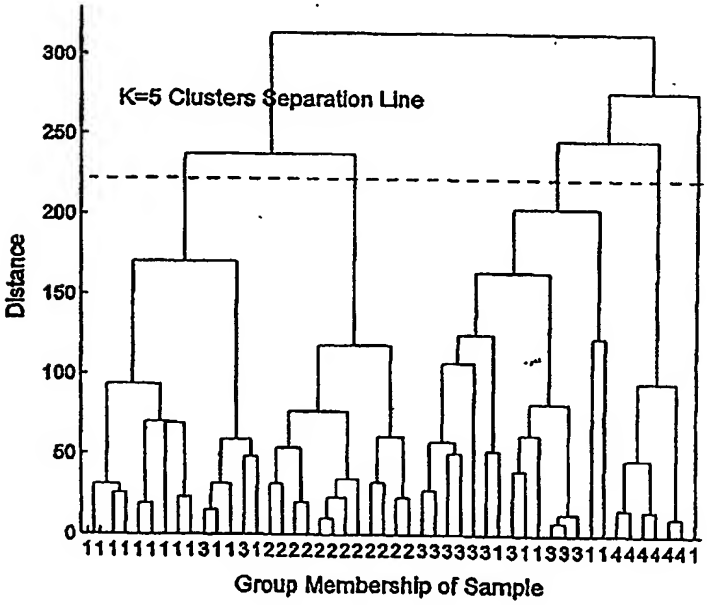

K=5 Clusters Separation Line
Distance
300
250
200
150
100
50
0
1111111113113122222222222233333331311393114444441
Group Membership of Sample

FIG. 9b

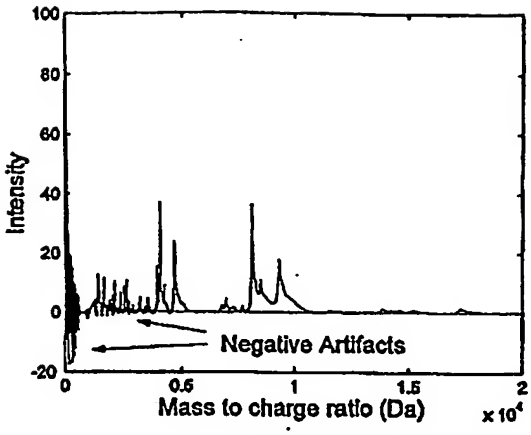

100
80
60
40
20
0
-20
Intensity
Negative Artifacts
0
0.5
1
1.5
2
Mass to charge ratio (Da)
x 10^4

FIG. 10

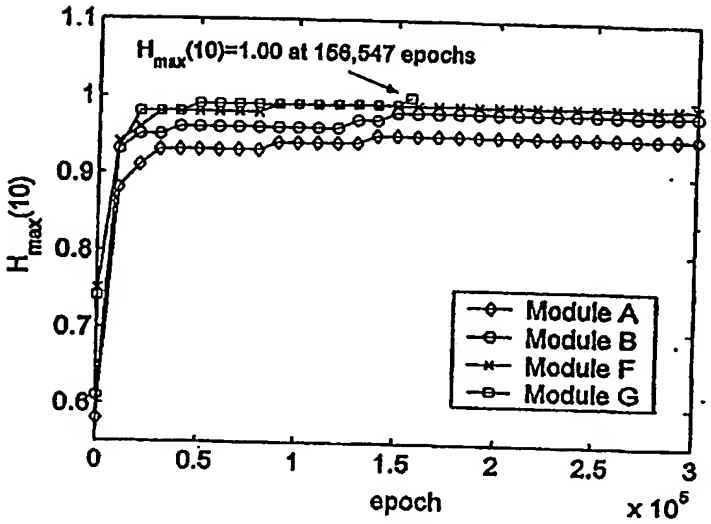

$H_{max}(10)$=1.00 at 166,547 epochs
$H_{max}(10)$
epoch
x $10^5$
Module A
Module B
Module F
Module G
1.1
1
0.9
0.8
0.7
0.6
0
0.5
1
1.5
2
2.5
3

FIG. 11